Optimization Algorithms for Parameter Estimation and Data Reconciliation

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Parameter Estimation and Data Reconciliation

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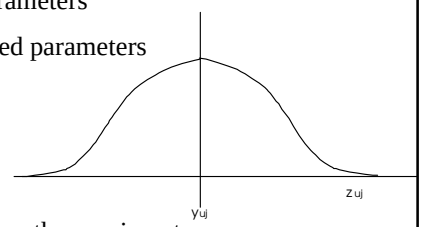
Maximum Likelihood Derivation - 1

Motivation:

- fit models to data to find 'optimal' parameters
- determine levels of confidence of fitted parameters
- evaluate suitability of models



Derivation of Objective Function

Let $z_{uj} = y_{uj}(\theta) + \varepsilon_{uj}$

z_{uj} - jth component of data for uth experiment

y_{uj} - corresponding (correct) model value

ε_{uj} - observation error following probability distribution function (pdf), p(z)

θ - adjustable parameters in model

What is p(z)? For a scalar z, how is it derived?

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Maximum Likelihood Derivation - 2

Assume the following moment information:

$$p(z) \geq 0, \int_{-\infty}^{\infty} p(z)dz = 1, \int_{-\infty}^{\infty} z\ p(z)dz = \eta, \int_{-\infty}^{\infty} (z-\eta)^2\ p(z)dz = \sigma^2$$

Define measure of information (Shannon, 1948) and find the distribution function that maximizes the information assuming only the moment information:

$$Max\ I(p) = E(\log p) = \int_{-\infty}^{\infty} \log(p(z))\, p(z)dz$$

$$s.t.\ p(z) \geq 0,\ \int_{-\infty}^{\infty} p(z)dz = 1$$

$$\int_{-\infty}^{\infty} z\ p(z)dz = \eta,\ \int_{-\infty}^{\infty} (z-\eta)^2\ p(z)dz = \sigma^2$$

Problem can be solved analytically to yield: $p(z) = \frac{1}{(\sqrt{2\pi})\sigma} \exp(-(z-\eta)^2/(2\sigma^2))$

If z is an m-vector for a single experiment, this can be extended to a joint multivariable distribution to give:

$$p(z) = (2\pi)^{-m/2} \det(V)^{-1/2} \exp(-1/2(z-\eta)^T (V)^{-1}(z-\eta))$$

where V is a covariance matrix defined by: $V = \int (z-\eta)(z-\eta)^T\ p(z)dz$

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Maximum Likelihood Derivation - 3

Consider n multiple experiments (with index u). Each experiment has a mean η_u, covariance V_u and experimental error distribution, ε_u

$$p(\varepsilon_u) = (2\pi)^{-m/2} \det(V)^{-1/2} \exp(-1/2(\varepsilon_u)^T (V)^{-1}(\varepsilon_u))$$

and the joint probability distribution is given by:

$$\prod_{u=1}^{n} p(\varepsilon_u) = (2\pi)^{-mn/2} \left[\prod_{u=1}^{n} \det(V_u)^{-1/2} \right] \exp(-1/2 \sum_{u=1}^{n} (\varepsilon_u)^T (V_u)^{-1}(\varepsilon_u))$$

This distribution now needs to be converted into an objective function that 'maximizes information' about our data.

Let's make the following assumptions:

- Replace distributional errors, ε_u by the actual residuals, $e_u = (z_u - y_u(\theta))$
- Experiments u are independent and V_u is the same for all experiments, $V = E(\varepsilon_u \varepsilon_u^T)$
- Define likelihood function $L(\theta) = \Pi\, p(e_u)$, and maximize this function (or its log).

This leads to the general form:

$$\log L(\theta) = -(nm/2)\log(2\pi) - (n/2)\log(\det(V)) - 1/2 \sum_{u=1}^{n} (e_u)^T (V)^{-1}(e_u)$$

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Maximum Likelihood Objective Functions

Specialize objectives based on what we know about the error distributions.

Define moment matrix:

$$M(\theta) = \sum_{u=1}^{n} (e_u)(e_u)^T, \; Tr(V^{-1}M(\theta)) = \sum_{u=1}^{n} (e_u)^T (V)^{-1}(e_u)$$

and $$\log L(\theta) = -(nm/2)\log(2\pi) - (n/2)\log(\det(V)) - 1/2 \sum_{u=1}^{n} Tr(V^{-1}M(\theta))$$

Since first two terms do not contain θ, we simply minimize $Tr(V^{-1} M(\theta))$

Special cases:

- <u>Ordinary Least Squares:</u> V is known, all component errors e_{uj} have same distribution and are independent of each other, i.e., V = v I

$$\text{Min } Tr(M(\theta)) = \Sigma_u \Sigma_j e_{uj}^2$$

- <u>Simple Weighted Least Squares:</u> V is known and diagonal, all component errors e_{uj} are independent of each other, i.e., $V = \text{diag}\{\sigma_j^2\}$

$$\text{Min } Tr(V^{-1}M(\theta)) = \Sigma_u \Sigma_j e_{uj}^2/\sigma_j^2$$

- <u>Weighted Least Squares:</u> V is known but general, all component errors e_{uj} depend on each other:

$$\text{Min } Tr(V^{-1}M(\theta)) = \Sigma_u \Sigma_j e_u^T V^{-1} e_u$$

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Maximum Likelihood – Unknown Covariance

Maximize L(θ) wrt V as well as θ.

$$\log L(\theta) = -(nm/2)\log(2\pi) - (n/2)\log(\det(V)) - 1/2\sum_{u=1}^{n} Tr(V^{-1}M(\theta))$$

Assuming V is symmetric and nonsingular, we get:

$$\frac{\partial \log L(\theta)}{\partial V} = -(n/2)V^{-1} - 1/2\sum_{u=1}^{n}(V^{-1}M(\theta)V^{-1}) = 0$$

which leads to: $V^* = 1/n\, M(\theta)$

Substitution into L(θ) leads to:

$$\log L(\theta) = -(nm/2)\log(2\pi) - (n/2)\log(n) - 1/2mn - n/2\log\det(M(\theta))$$

so we minimize: $n/2 \log \det(M(\theta))$

Notes:

- If the structure of V is known, we can further specialize the objective for unknown covariance (e.g., diagonal covariance, same covariance)
- V* is biased but can be corrected by using V" = n/(n-m n_θ) V*

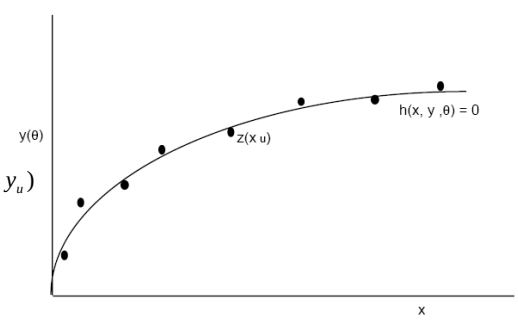
Unconstrained Least Squares

Basic Problem:

$$Min\ \Phi(\theta, y, z) = 1/2\sum_{u=1}^{n}(z_u - y_u)^T W_u (z_u - y_u)$$

$$s.t.\ \ h_u(x_u, y_u, \theta) = 0$$

$$a \le \theta \le b$$



- W_u can be chosen to be $(V_u)^{-1}$
- $h_u(x_u, y_u, \theta) = 0$ is a model of the system
- x_u are fixed independent variables
- Bounds are not expected to be active

Consider the case where y_u is an explicit function of θ,

$$h_u(x_u, y_u, \theta) = 0 \implies y_u = f_u(x_u, \theta)$$

and $$Min\ \Phi(\theta, y, z) = 1/2\sum_{u=1}^{n}(z_u - f_u(\theta))^T W_u (z_u - f_u(\theta))$$

Least Squares – Solution Methods

Linear Least Squares

Model is given by: $y_u = A_u\theta + b_u$

$$Min\ \Phi(\theta, z) = 1/2\sum_{u=1}^{n}(z_u\text{-}A_u\theta - b_u)^T W_u (z_u\text{-}A_u\theta - b_u)$$

From $\nabla_\theta \Phi(\theta, z) = 0$, we get the normal equation:

$$\sum_{u=1}^{n}(A_u{}^T W_u A_u)\theta = \sum_{u=1}^{n} A_u{}^T W_u (z_u - b_u)$$

and this leads to: $\theta = \left(\sum_{u=1}^{n}(A_u{}^T W_u A_u)\right)^{-1}\sum_{u=1}^{n} A_u{}^T W_u (z_u - b_u)$

Note: A better way to solve this linear system is to do a QR factorization on a concatenation (over u) of $(Wu)^{1/2}A_u$.

Least Squares – Solution Methods

Nonlinear Least Squares

Model is given by: $y_u = f_u(x_u\theta)$

$$Min\ \Phi(\theta, z) = 1/2\sum_{u=1}^{n}(z_u\text{-}f_u(\theta))^T W_u (z_u\text{-}f_u(\theta))$$

And we solve this unconstrained problem with Newton's method

From Taylor series expansion: $\nabla_\theta \Phi(\theta^k, z) + \nabla_{\theta\theta}\Phi(\theta^k, z)\Delta\theta = 0$

$$\nabla_\theta \Phi(\theta^k, z) = -\sum_{u=1}^{n} J_u^T W_u (z_u - f_u(\theta^k)),\ J_u = \nabla_\theta f_u{}^T$$

$$\nabla_{\theta\theta}\Phi(\theta^k, z) = \sum_{u=1}^{n}(J_u^T W_u J_u + R_u),\ \{R_u\}_{ij} = -\nabla_{\theta_i\theta_j} f_u^T W_u (z_u - f_u(\theta^k))$$

Now assume that $(z_u\text{-}f_u(\theta))$ is nearly zero and therefore R_u is nearly zero. Then the Hessian simplifies to: $\nabla_{\theta\theta}\Phi(\theta^k, z) = \sum_{u=1}^{n} J_u^T W_u J_u$

and we have the **Gauss-Newton Method**:

$$\Delta\theta = \left(\sum_{u=1}^{n}(J_u{}^T W_u J_u)\right)^{-1}\sum_{u=1}^{n} J_u{}^T W_u (z_u - f_u(\theta^k))$$

Note: A better way to solve this linear system is to do a QR factorization on a concatenation (over u) of $(W_u)^{1/2}J_u$.

Globalization of Gauss-Newton Method

To ensure convergence from poor starting points:

<u>Line search method</u>

Choose $\alpha \in (0, 1]$ so that a sufficient decrease is found for $\Phi(\theta)$ with: $\theta^{k+1} = \theta^k + \alpha\, \Delta\theta$.

This will converge to a stationary point ($\nabla_\theta \Phi = 0$) as long as

$\sum_{u=1}^{n} J_u^T W_u J_u$ is sufficiently positive definite. What if singular?

Add λ I to Hessian to get the **<u>Levenberg-Marquardt method</u>**.

$$\Delta\theta = \left(\sum_{u=1}^{n} (J_u{}^T W_u J_u) + \lambda I \right)^{-1} \sum_{u=1}^{n} J_u{}^T W_u (z_u - f_u(\theta^k))$$

How should λ be adjusted?

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Unconstrained Problems: TR Motivation

Take: $Min \quad \Phi(\theta)$

Model Problem: $Min \quad \Phi(\theta_k) + \nabla\Phi(\theta_k)^T \Delta\theta + \frac{1}{2}\Delta\theta \nabla^2\Phi(\theta_k)^T \Delta\theta$

$$\frac{1}{2}\|\Delta\theta\|^2 \le \frac{1}{2}\Delta^2$$

Optimality Conditions: Leads to Levenberg-Marquardt Method

$$\left\{ \begin{array}{c} \nabla\Phi(\theta_k) + \nabla^2\Phi(\theta_k)^T \Delta\theta + \lambda\Delta\theta = 0 \\ \|\Delta\theta\|^2 \le \Delta^2, \lambda \ge 0 \\ \lambda(\|\Delta\theta\|^2 - \Delta^2)/2 = 0 \end{array} \right\} \Longrightarrow \Delta\theta = -(\nabla^2\Phi(\theta_k) + \lambda I)^{-1} \nabla\Phi(\theta_k)$$

How do we choose λ or Δ?

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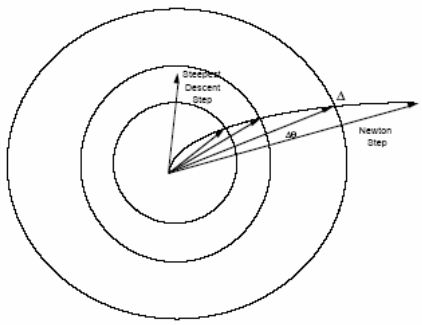
Extremes of Trust Region Method



For given Δ, solve for λ directly

$$1/||\Delta\theta(\lambda)|| - 1/\Delta = 0$$

$\lambda = 0$, Δ large: $\Delta\theta$ is the Gauss-Newton Step

$\lambda \dashrightarrow \infty$, $\Delta = 0$: $\Delta\theta$ is a small step in the steepest descent direction

Trust Region Methods - guaranteed to converge to local optima, with much weaker assumptions than line search methods.

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Trust region approach in MINPACK (More', 1980)

Choose λ so that $\| \Delta\theta \| \leq \Delta$, comparing τ = ared/pred

- actual reduction (ared): $\Phi(\theta^k) - \Phi(\theta^k + \Delta\theta)$
- predicted reduction (pred): $\nabla_{\theta\theta}\Phi^T\Delta\theta + 1/2\, \Delta\theta^T\nabla_{\theta\theta}\Phi\, \Delta\theta$

At iteration k:

- Calculate λ corresponding to Δ, and calculate $\Delta\theta$.
- Evaluate (ared) and (pred).
- Define τ = ared/pred

  a) If $\rho_1 < \tau \leq \rho_0$, $\Delta = m_1 \Delta$

  b) If $\rho_2 \leq \tau < \rho_1$ or $\rho_0 < \tau$, $\Delta = \Delta$

  b) If $\tau < \rho_2$, $\Delta = \Delta / m_1$

  c) If $\tau < \rho_3$ reset $\Delta\theta = 0$

  Set, $\theta^{k+1} = \theta^k + \Delta\theta$

Typical values for the parameters:

$m_1 = m_2 = 2$ and $\rho_1 = 0.75$, $\rho_2 = 0.25$, $\rho_3 = 0$, $\rho_0 = 2$.

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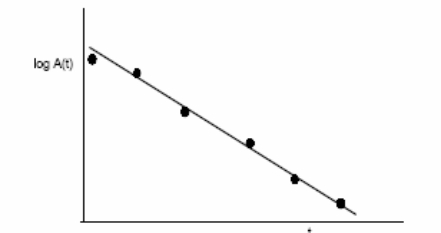
Why is trust region required for parameter estimation?



First order reaction: $A(t) = A(0) \exp(-k\, t)$; $k = k_0 \exp(-E/RT)$

Data available only at one temperature.

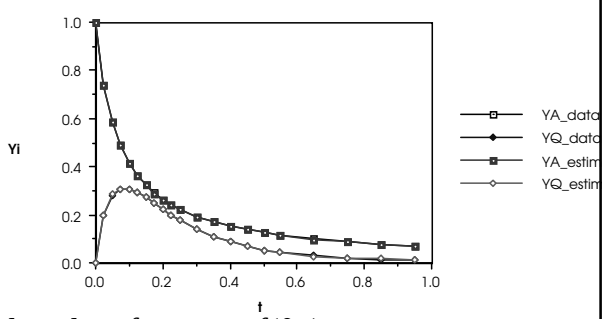
<u>Results:</u>

- Nonunique parameter estimates, k_0, E
- Singular Hessian
- Can be due to poor model and/or poor data
- Trust region methods will ensure convergence to "some" solution,
- Postoptimality analysis will establish nonuniqueness, insensitivity

Example: Catalytic Cracking of Gasoil (Tjoa, 1991)

$$A \xrightarrow{k_1} Q \xrightarrow{k_2} S, \quad A \xrightarrow{k_3} S$$

$$y_A' = -(k_1+k_3)\, y_A^2$$
$$y_Q' = -k_1 y_A^2 - k_2\, y_Q$$
$$y_A(0) = 1,\ y_Q(0) = 0$$



ODEs can be solved to yield explicit form: $y = f(\theta,t)$

Apply Trust Region method (GREG):

$(k_1, k_2, k_3)_0 = (6, 4, 1)$

$(k_1, k_2, k_3)_* = (11.95, 7.99, 2.02)$

$(k_1, k_2, k_3)_{true} = (12, 8, 2)$

Converges in 5 iterations (11 function calls)

Convergence Rates for Gauss-Newton Methods

Small Residuals at Solution (Good Model Fit):

$e_u^* = 0$, $R_u^* = 0$,

$$\nabla_{\theta\theta}\Phi(\theta^*,z) = \sum_{u=1}^{n} J_u^T W_u J_u$$

- Gauss-Newton method is quadratically convergent.
- Trust region will be inactive if Hessian is nonsingular
- L-M is also quadratically convergent for unique θ^*.

Large Residuals at Solution (Poor Model Fit):

$e_u^* \neq 0$, $R_u^* \neq 0$,

$$\nabla_{\theta\theta}\Phi(\theta^*,z) = \sum_{u=1}^{n} J_u^T W_u J_u + R_u$$

- Gauss-Newton method is linearly convergent.
- Trust region may not be inactive if Hessian is nonsingular
- L-M is also linearly convergent for unique θ^*.

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Hybrid Methods (Gauss and quasi-Newton)

Quasi-Newton Methods

- DFP and BFGS Methods apply secant formula, symmetry and positive definiteness of Hessian
- Do not exploit structure of least squares problem

Dennis, Gay and Welsh (1981) - NL2SOL

- Approximates true Hessian as G-N Hessian is known
- Specialized, self-scaling Q-N method developed that approximates R_u
- Incorporates Trust Region Approach of More'
- Leads to superlinear convergence

Fletcher and Xu (1987)

- Applies specialized Q-N method to approximate R_u
- Uses a switching rule to monitor if there are small or large residuals

$$\tau^k = (\Phi(\theta^k) - \Phi(\theta^{k+1}))/\Phi(\theta^k)$$

Large residuals: $\lim_{k\to\infty} \tau^k = 0$, Use specialized Q-N update if $\tau^k \leq \varepsilon$

Small residuals: $\lim_{k\to\infty} \tau^k = 1$, Use specialized G-N formula if $\tau^k > \varepsilon$

(Choose $\varepsilon \sim 0.1$)

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Constrained Least Squares

Motivation:

- Model cannot be reformulated as $y = f(\theta)$
- Too expensive to converge $h_u(y_u, \theta) = 0$ for each parameter value

Basic Formulation:

$$Min\ \Phi(\theta, y, z) = 1/2 \sum_{u=1}^{n} (z_u - y_u)^T W_u (z_u - y_u)$$
$$s.t.\ \ h_u(y_u, \theta) = 0$$
$$a \le \theta \le b$$

- Any NLP method can be used to solve this problem
- SQP can be tailored to take advantage of special form of Φ allows for tailored algorithm.
- Leads to faster algorithm than standard SQP with BFGS updates

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Optimization Strategy: SQP method

Let $x^T = [\theta^T, y^T]$ and consider QP subproblems for SQP:

$$\min \quad \nabla\Phi(x^k)^T d + 1/2\, d^T B\, d$$
$$\text{s.t. } h(x^k) + \nabla h(x^k)^T d = 0$$
$$x^L \le x^k + d \le x^U$$

First order necessary conditions

$$\begin{bmatrix} B & \nabla h \\ \nabla h^T & 0 \end{bmatrix} \begin{bmatrix} d \\ v \end{bmatrix} = - \begin{bmatrix} \nabla\Phi \\ h \end{bmatrix}$$

Problems:

- How to deal with a larger QP problems
- How to calculate the Hessian

Strategies:

- Use Range and Null space Decomposition strategy to decompose the search direction into:
  - Null space movement
  - Range space movement
- Use a hybrid Gauss-Newton and BGFS update formula
- Analogy to unconstrained approaches

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Range and Null Space Decomposition

Define linear QP system as: M s = f, to give:

$$\begin{bmatrix} B & \nabla h \\ \nabla h^T & 0 \end{bmatrix} \begin{bmatrix} d \\ v \end{bmatrix} = - \begin{bmatrix} \nabla \Phi \\ h \end{bmatrix}$$

and select an n x n nonsingular matrix: H = [Y | Z], where $\nabla h^T Z = 0$.

- Z, Y are null & range space bases for the linearized equalities
- Search direction with range (p_Y) and null space (p_Z) components:

$$d = Y p_Y + Z p_Z. \quad Y^T = [\ 0 \mid I\ ] \qquad Z^T = [\ I \mid N^T C^{-T}]$$

Now defining X = diag [[Y | Z] , I], we can consider the equivalent system $X^T M X z = X^T f$ (with X z = s) as:

$$\begin{bmatrix} Y^T BY & Y^T BY & Y^T \nabla h \\ Z^T BY & Z^T BZ & 0 \\ \nabla h^T Y & 0 & 0 \end{bmatrix} \begin{bmatrix} p_Y \\ p_Z \\ v \end{bmatrix} = - \begin{bmatrix} Y^T \nabla \Phi \\ Z^T \nabla \Phi \\ h \end{bmatrix}$$

Standard assumptions: set $Y^T B\, Y = 0$ and $Y^T B\, Z = 0$

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Structure of Least Squares Hessian

$$B^k = \begin{bmatrix} \nabla_{\theta\theta} L & \nabla_{\theta y} L \\ \nabla_{y\theta} L & \nabla_{yy} L \end{bmatrix}$$

$$\nabla_{\theta\theta} L = \sum_{j=1}^{m} v_j \nabla_{\theta\theta} h_j \qquad \nabla_{\theta y} L = \sum_{j=1}^{m} v_j \nabla_{\theta y} h_j$$

$$\nabla_{y\theta} L = \sum_{j=1}^{m} v_j \nabla_{y\theta} h_j \qquad \nabla_{yy} L = \nabla_{yy} \Phi + \sum_{j=1}^{m} v_j \nabla_{yy} h_j$$

where $L(\theta, y, v) = \Phi(y) + v^T h(\theta, y)$

KKT multipliers (based on first order estimates) are given by:

$$v = - (Y^T \nabla h)^{-1} Y^T \nabla \Phi = - (Y^T \nabla h)^{-1} Y^T\ [\ 0 \mid \Sigma_u e_u^T W_u]^T$$

Assumption: If the residuals are *small*, then at convergence $e_u \approx 0 \Rightarrow v \approx 0$

The Hessian becomes $B^{G\text{-}N} = \begin{bmatrix} 0 & 0 \\ 0 & (W_u) \end{bmatrix}$

$\Rightarrow$ *Newton-like* rate of convergence

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Least Squares Hybrid SQP Method

Motivation: Choose best Hessian approximation for different problem types

Strategies: Develop a switching rule to decide if Q-N or G-N approximation should be made for B^k. (Fletcher and Xu, 1987)

- Define merit function: $L^*(x^k) = \Phi(x^k) + v^T h(x^k) + 1/2\, \gamma\, \|h(x^k)\|^2$
- Uses a switching rule to monitor if there are small or large residuals

$$\tau^k = (L^*(x^k) - L^*(x^{k+1}))/L^*(x^k)$$

Large residuals: $\lim_{k \to \infty} \tau_k = 0$, Use specialized Q-N for $Z^T B Z$ if $\tau_k \leq \varepsilon$

Small residuals: $\lim_{k \to \infty} \tau_k = 1$, Use $Z^T B^{GN} Z$, $Z^T B^{GN} Y p_Y$ formula, $\tau_k > \varepsilon$

Choose $\varepsilon \sim 0.2$

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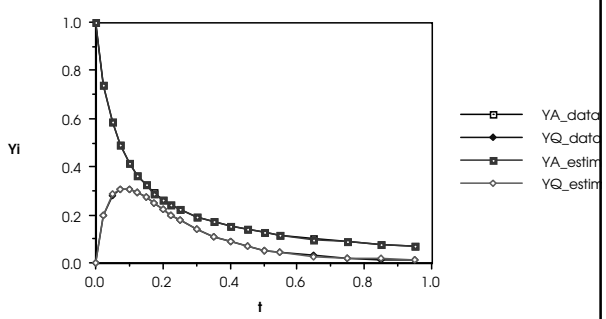
Example: Catalytic Cracking of Gasoil (Tjoa, 1991)

$$A \xrightarrow{k_1} Q \xrightarrow{k_2} S, \quad A \xrightarrow{k_3} S$$

$$y_A' = -(k_1+k_3)\, y_A^2$$
$$y_Q' = -k_1 y_A^2 - k_2\, y_Q$$
$$y_A(0) = 1,\ y_Q(0) = 0$$



number of ODEs: 2
number of parameters: 3
discretized ODEs: 68 variables

$(k_1, k_2, k_3)_0 = (6, 4, 1)$
$(k_1, k_2, k_3)_* = (11.95, 7.99, 2.02)$
$(k_1, k_2, k_3)_{true} = (12, 8, 2)$

Method	Obj.	Iters.	CPU (s, V3200)
BFGS SQP	8.23e-5	10	4.31
Gauss-Newton	8.23e-5	4	2.25
Hybrid SQP	8.23e-5	4	2.31

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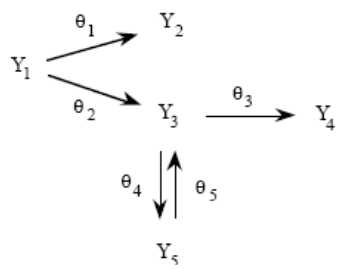
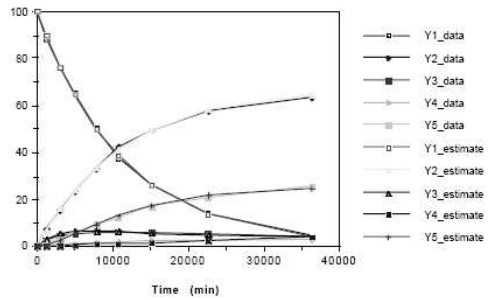
Small Residual Example: α-Pinene Kinetics





number of ODEs: 5
number of parameters: 5
discretized ODEs: 245 variables

Method	Iters.	CPU (s, V3200)
BFGS SQP	37	90.8
MINOS	21	64.8
Gauss-Newton	6	23.5
Hybrid SQP	6	23.6

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Further Results (Tjoa and Biegler,1990)

Number of Iterations (Function Evaluations)

Problem	GREG	MINOS	SQP based methods		
			BFGS	GN	Hybrid
1	6 (12)	8 (41)	8 (10)	3 (3)	3 (3)
2	14 (34	8 (72)	14 (17)	3 (3)	3 (3)
3	6 (12)	8 (55)	30 (31)	3 (3)	3 (3)
4	7 (20)	13 (95)	14 (15)	6 (6)	6 (6)
5	7 (19)	15 (236)	fail	13 (16)	13 (16)
6	5 (10)*	7 (72)	13 (21)	5 (5)	5 (5)
7	8 (16)	10 (150)	24 (30)	5 (5)	6 (6)
8	fail	21 (271)	37 (61)	6 (6)	6 (6)
9	26 (95)*	33 (320)	19 (24)	fail	18 (18)

*: using least squares objective function

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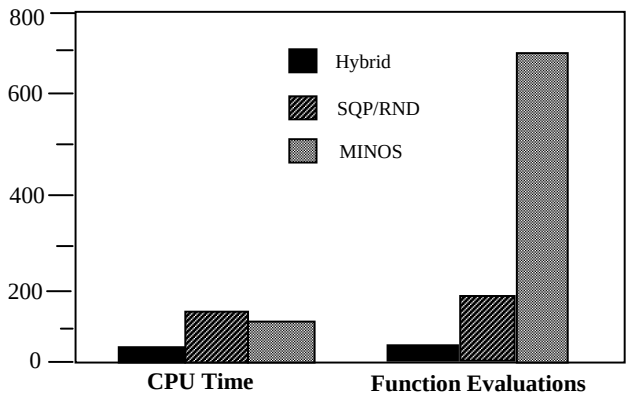
Comparison of Hybrid vs. General Purpose NLP Codes (Tjoa)



- Summary on 10 parameter estimation (kinetics) problems
- Few parameters, degrees of freedom
- Hybrid method for Hessian structure:
  (Fletcher and Xu) quasi-Newton method.

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Further Comparison – Constrained Trust Region Method (Arora, 2003)

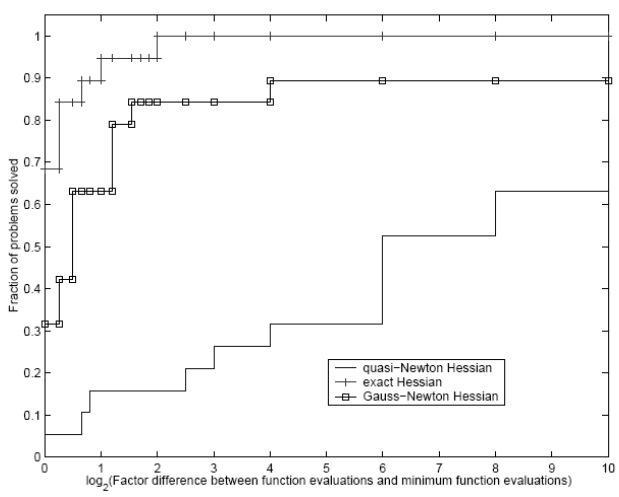

Figure 4.8: Parameter Estimation Problems

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Statistical Inference of Estimated Parameters

Covariance of Optimal Parameters

Given an error distribution for the data (assumed Gaussian with covariance, V_z)
How does this affect the accuracy of the estimated parameters?

Recall: $V_z = E(\delta z\ \delta z^T)$ *and* $V\theta = E(\delta\theta^*\ \delta\theta^{*T})$

How does θ change with data z?

$$i.e.,\ \frac{\partial\Phi(\theta^*,z)}{\partial\theta}=0,\quad \frac{\partial\Phi(\theta^*+\delta\theta,z+\delta z)}{\partial\theta}=0$$

$$Approximate\ by: \frac{\partial\Phi^2(\theta^*,z)}{\partial\theta\,\partial z}\delta z+\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta^2}\delta\theta=0$$

$$and\quad \delta\theta=\left[\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta^2}\right]^{-1}\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta\,\partial z}\delta z,\ so\ we\ have:$$

$$V_\theta=E(\delta\theta\,\delta\theta^T)=\left[\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta^2}\right]^{-1}\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta\,\partial z}E(\delta z\,\delta z^T)\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta\,\partial z}^T\left[\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta^2}\right]^{-T}$$

$$\Rightarrow V_\theta=\left[\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta^2}\right]^{-1}\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta\,\partial z}V_z\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta\,\partial z}^T\left[\frac{\partial\Phi^2(\theta^*,z)}{\partial\theta^2}\right]^{-T}$$

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Special Cases for Covariance

1. If the objective function has covariance independent of u, i.e.:

$$\Phi=\sum_{u=1}^{n}(z_u-f_u(\theta))^TV_z^{-1}(z_u-f_u(\theta))\ \text{ then we have: } V_\theta=\sum_{u=1}^{n}(J_u{}^TV_z^{-1}J_u)^{-1}$$

2. If z_u is a scalar, then V_z is σ^2 and V_θ is given by: $\sigma^2\sum_{u=1}^{n}\left(\frac{\partial f_u}{\partial\theta}\frac{\partial f_u}{\partial\theta}^T\right)^{-1}$

3. If the covariance for z is unknown, then estimate from moment matrix $V_z = M(\theta)/n$ and then: $V_\theta=\sum_{u=1}^{n}(J_u{}^TV_z^{-1}J_u)^{-1}$

4. For general likelihood functions, $V_\theta = -(\nabla_{\theta\theta}(\log L(\theta^*))^{-1}$ is asymptotically correct as $n \rightarrow \infty$.

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Elliptical Confidence Regions

Single parameter

For a given interval let $\gamma = \Pr(a \le \theta^* \le b) = \int_a^b p(\theta^*|\theta_{true})\, d\theta$

and for a single parameter this becomes: $|\theta_{true} - \theta^*| \le \zeta$ where ζ is the confidence level for γ with σ_θ calculated with n --> ∞ and

$$\sigma_\theta^2 = \sigma^2 \sum_{u=1}^{n} \left(\frac{\partial f_u}{\partial \theta} \frac{\partial f_u}{\partial \theta}^T \right)^{-1}$$

Otherwise, with a small sample size: $|\theta_{true} - \theta^*| \le t\, s_\theta$

$$s = \frac{1}{n-1}\left[\sum_{u=1}^{n}(z_u - f_u(\theta))^2\right]^{-1} \qquad s_\theta^2 = s^2 \sum_{u=1}^{n} \left(\frac{\partial f_u}{\partial \theta} \frac{\partial f_u}{\partial \theta}^T \right)^{-1}$$

Multiple parameters

Map out a region $S(\theta)$ so that $\gamma = \Pr(\theta_{true} \in S(\theta))$

This can be done using the principal directions of V_θ which leads to:

$$\gamma = \Pr((\theta_{true}-\theta^*)^T V_\theta^{-1} (\theta_{true}-\theta^*))$$

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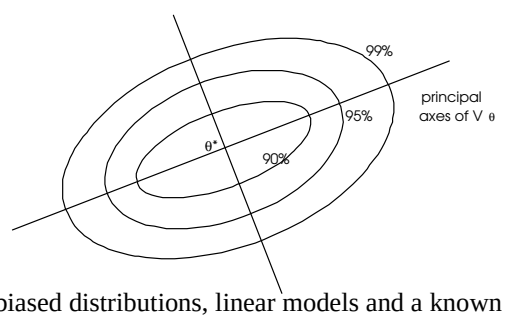

For normal, unbiased distributions, linear models and a known V_θ, this probability follows a χ^2 distribution so that the region can be defined by:

$$(\theta_{true}-\theta^*)^T V_\theta^{-1} (\theta_{true}-\theta^*) \le c(\gamma)$$

$c(\gamma)$ is χ^2 value for γ level of confidence with n_θ degrees of freedom.

- For a scalar z, the χ^2 test simplifies to an F-test for determination of $c(\gamma)$.
- Elliptical confidence regions are correct if the model is linear or for small levels of confidence, γ. Otherwise, confidence regions can deviate greatly from ellipses.
- Elliptical confidence regions are most commonly used. Nonlinear confidence regions much more expensive to calculate.

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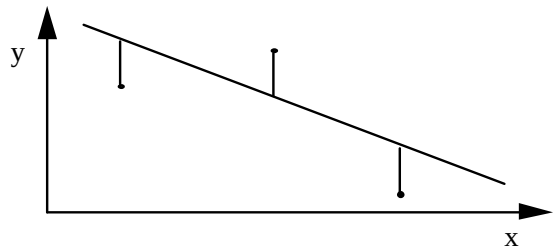
Errors in Variables Models (EVM)

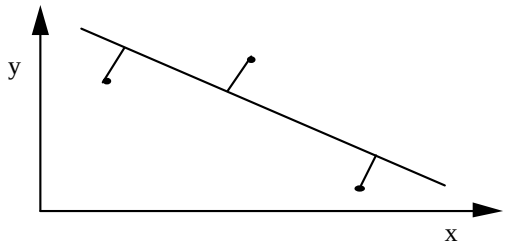
Conventional model: $y = f(x,\theta)$ or $h(x, y, \theta) = 0$



No. of independent variables (x) = s_1
No. of dependent variables (y) = s_2
No. of parameters (θ) = p
No. of constraints = m
No. of data sets = r
$\Rightarrow$ *No error in the "independent" variables, x*
Number of degrees of freedom for optimization = p
Minimize vertical distance, e.g. $(y_u - z_u)^2$

Errors in Variables Models (EVM) - 2

Implicit Model: $f(x,y,\theta) = 0$
Both x and y have inherent measurement errors
$\Rightarrow$under-determined system
(e.g., pressure vs. temperature data)



Number of degrees of freedom for optimization
= p + (s-m)r
$\Rightarrow$ NLP size grows linearly with the number of data sets
Minimize a *nonvertical* distance

EVM Problem Statement

$$Min\ \ \Phi = 1/2\sum_{u=1}^{r} e_u^T W e_u$$
$$s.t.\ \ f_u(w_u, \theta) = 0$$
$$a \le \theta \le b$$
where $e_u = w_u - z_u,\ w_u^T = [x_u^T\ y_u^T]$

$$Min\ \ \Phi = \sum_{u=1}^{r} \phi_u = 1/2\sum_{u=1}^{r} e_u^T W e_u$$
$$s.t.\ \ h_u(w_u, \zeta_u, \theta) = 0$$
$$a \le \theta \le b$$
where $h_u^T = [\,f_u^T\ g_u^T\,]$

Formulation:
- Least squares nonlinear constraints with many degrees of freedom

Current Approaches
- Nonlinear Programming Strategies – Expensive if sparsity not exploited
- Linearized Least Squares - Not robust, global convergence not enforced

Introduce
New variables: ζ_u
New constraints: $g_u = \zeta_u - \theta = 0$.

Solution Strategy:
- Apply decoupling strategy to SQP method
- Decompose for each data set
- Computational cost linear in # of data sets
- Can solve in parallel

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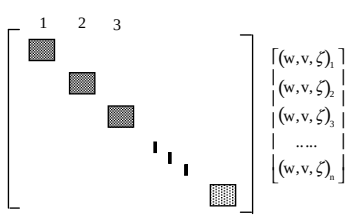
KKT Conditions for EVM

Structure of the KKT matrix after decoupling:



= RHS(Δθ)

$$\begin{bmatrix} B_u & \nabla h_u \\ \nabla h_u^T & 0 \end{bmatrix}\begin{bmatrix} d_u \\ v_u \end{bmatrix} = -\begin{bmatrix} \nabla \phi_u \\ h_u \end{bmatrix} \quad \nabla h_u = \begin{bmatrix} \nabla_w f_u & 0 \\ \nabla_\zeta f_u & I \end{bmatrix} \quad d = \begin{bmatrix} \Delta w_u \\ \Delta \zeta_u \end{bmatrix} \quad v_u = \begin{bmatrix} \lambda_u \\ \gamma_u \end{bmatrix}$$

Once θ is fixed, can solve for remaining variables independently.

Can exploit each KKT system further.

Structure of Hessian (Gauss-Newton): $B_u = \begin{bmatrix} W_u & 0 \\ 0 & 0 \end{bmatrix}$

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EVM Decomposition

$$\begin{bmatrix} B_u & \nabla h_u \\ \nabla h_u^T & 0 \end{bmatrix} \begin{bmatrix} d_u \\ v_u \end{bmatrix} = -\begin{bmatrix} \nabla \phi_u \\ h_u \end{bmatrix}$$

<u>Apply Range and Null space Decomposition</u>

- Subspace search directions: $\nabla h_u^T Z_u = 0$, $Y_u^T Z_u = 0$
- Define: $d_u = Z_u p_{Z,u} + Y_u p_{Y,u}$

  Null space step: $p_{Z,u} = -(Z_u^T B_u^{GN} Z_u)^{-1} Z_u^T \nabla \phi_u$

  Range space step: $p_{Y,u} = -(\nabla h_u^T Y_u)^{-1} h_u$
- Note: $p_{Y,u}$ is dependent on $\Delta\theta$, $p_{Z,u}$ is not!

<u>Reconstruct QP Problem is space of $\Delta\theta$</u>

- Sum up contributions from all data sets

$$\underset{\Delta\theta}{Min} \left(\sum_{u=1}^{r} \alpha_u \right)^T \Delta\theta + 1/2\, \Delta\theta^T \left(\sum_{u=1}^{r} \beta_u \right) \Delta\theta$$

$$s.t. \quad a\text{-}\theta^k \le \Delta\theta \le b\text{-}\theta^k$$

where α_u and β_u are derived from ∇h_u

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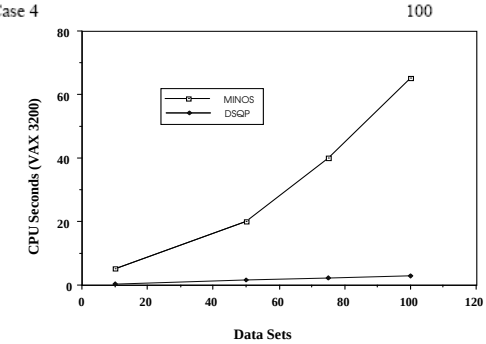
EVM Examples

Example	Model	Number of Data sets	d.o.f
1	$y = \theta_1 + \theta_2 x$	10	12
2	$y = \theta_1 + \theta_2 x + \theta_3 x^2 + \theta_4 x^3$	10	14
3	$\exp(-\theta_1 t \exp(-\theta_2/T)) - y = 0.$	15	32
4	$x_3 = \dfrac{\theta_1 \theta_2^2 \theta_3 x_1 x_2^3}{(1+\theta_1 x_1 + \theta_2 x_2)^3}$	28	59
5, Case 1	$x_2 = \theta_1 + \dfrac{1}{x_1 - \theta_2}$	25	27
5, Case 2		50	52
5, Case 3		75	77
5, Case 4		100	102



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Full-space NLP Formulation for Parameter Estimation

Original Formulation

$$\min_{x \in \Re^n} f(x)$$
$$\text{s.t} \quad c(x) = 0$$
$$x \geq 0$$

Can generalize for

$$a \leq x \leq b$$

Barrier Approach

$$\min_{x \in \Re^n} \varphi_\mu(x) = f(x) - \mu \sum_{i=1}^{n} \ln x_i$$
$$\text{s.t} \quad c(x) = 0$$

$\Rightarrow$As $\mu \rightarrow 0$, $x^*(\mu) \rightarrow x^*$

Fiacco and McCormick (1968)

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Solution of the Barrier Problem - IPOPT

$\Rightarrow$**Newton Directions (KKT System)**

$$\begin{aligned} \nabla f(x) + A(x)\lambda - v &= 0 \\ XVe - \mu e &= 0 \\ c(x) &= 0 \end{aligned}$$

$\Rightarrow$ **Reducing the System**

$$d_v = \mu X^{-1} e - v - X^{-1} V d_x$$

$$\begin{bmatrix} Q+\Sigma & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} d_x \\ \lambda^+ \end{bmatrix} = -\begin{bmatrix} \nabla \varphi_\mu \\ c \end{bmatrix} \qquad \Sigma = X^{-1} V$$

What are the Benefits for Parameter Estimation?

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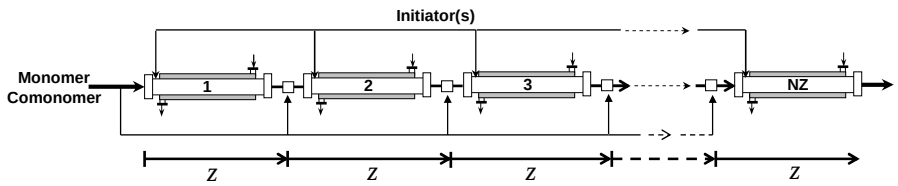
Large-Scale Parameter Estimation



Material & Energy

Physical Properties

Zone Transitions

$$\left.\begin{cases} \mathbf{F}_j\left[\dfrac{dy_j(z)}{dz}, y_j(z), w_j(z), z, \pi_j, \Pi\right] = 0 \\ \mathbf{G}_j\left[y_j(z), w_j(z), z, \pi_j, \Pi\right] = 0 \\ y_j(0) = \phi(y_{j-1}(z_{L_{j-1}}), F_{f_j}) \end{cases}\right\} j \in \{1..NZ\}$$

500 ODEs
1000 AEs

× **Stiffness + Highly Nonlinear + Parametric Sensitivity + Algebraic Coupling**

Large-Scale Parameter Estimation

- **Complex Kinetic Mechanisms**

Initiator decomposition

$$I_i \xrightarrow{k_{d_i}} 2R \quad i = 1, N_I$$

Chain Initiation

$$R + M_1 \xrightarrow{k_{I_1}} P_{1,0}$$
$$R + M_2 \xrightarrow{k_{I_2}} Q_{0,1}$$

Chain Propagation

$$P_{r,s} + M_1 \xrightarrow{k_{p11}} P_{r+1,s}$$
$$P_{r,s} + M_2 \xrightarrow{k_{p12}} Q_{r,s+1}$$
$$Q_{r,s} + M_1 \xrightarrow{k_{p21}} P_{r+1,s}$$
$$Q_{r,s} + M_2 \xrightarrow{k_{p22}} Q_{r,s+1}$$

Chain Transfer to Monomer

$$P_{r,s} + M_1 \xrightarrow{k_{fm11}} P_{1,0} + M_{r,s}$$
$$P_{r,s} + M_2 \xrightarrow{k_{fm12}} Q_{0,1} + M_{r,s}$$
$$Q_{r,s} + M_1 \xrightarrow{k_{fm21}} P_{1,0} + M_{r,s}$$
$$Q_{r,s} + M_2 \xrightarrow{k_{fm22}} Q_{0,1} + M_{r,s}$$

Chain Transfer to Solvent

$$P_{r,s} + S_i \xrightarrow{k_{si1}} P_{1,0} + M_{r,s}$$
$$Q_{r,s} + S_i \xrightarrow{k_{si2}} Q_{0,1} + M_{r,s}$$

Chain Transfer to Polymer

$$P_{r,s} + M_{x,y} \xrightarrow{k_{fp11}} P_{x,y} + M_{r,s}$$
$$P_{r,s} + M_{x,y} \xrightarrow{k_{fp12}} Q_{x,y} + M_{r,s}$$
$$Q_{r,s} + M_{x,y} \xrightarrow{k_{fp21}} P_{x,y} + M_{r,s}$$
$$Q_{r,s} + M_{x,y} \xrightarrow{k_{fp22}} Q_{x,y} + M_{r,s}$$

Termination by Combination

$$P_{r,s} + P_{x,y} \xrightarrow{k_{tc11}} M_{r+x,s+y}$$
$$P_{r,s} + Q_{x,y} \xrightarrow{k_{tc12}} M_{r+x,s+y}$$
$$Q_{r,s} + Q_{x,y} \xrightarrow{k_{tc22}} M_{r+x,s+y}$$

Termination by Disproportionation

$$P_{r,s} + P_{x,y} \xrightarrow{k_{td11}} M_{r,s} + M_{x,y}$$
$$P_{r,s} + Q_{x,y} \xrightarrow{k_{td12}} M_{r,s} + M_{x,y}$$
$$Q_{r,s} + Q_{x,y} \xrightarrow{k_{td22}} M_{r,s} + M_{x,y}$$

Backbitting

$$P_{r,s} \xrightarrow{k_{b1}} P_{r,s} \ or \ Q_{r,s}$$
$$P_{r,s} \xrightarrow{k_{b2}} Q_{r,s} \ or \ P_{r,s}$$

β-scission

$$P_{r,s} \xrightarrow{k_{\beta 1}} M^{=}_{r,s} + P_{1,0}$$
$$P_{r,s} \xrightarrow{k_{\beta 2}} M^{=}_{r,s} + Q_{0,1}$$

$$k = k_0 \, exp\left(-\frac{E_a + P\,E_v}{RT}\right)$$

~ 35 Elementary Reactions
~100 Kinetic Parameters

Large-Scale Parameter Estimation

- **Parameter Estimation for Industrial Applications**
  - **Use Rigorous Model to Match Plant Data Directly**
  - **Start with Standard Least-Squares Formulation**

$$\min_{\Pi,\pi_{k,j}} \sum_{k=1}^{NS}\sum_{j=1}^{NZ}\sum_{i=1}^{NM(j)} \left(y_{k,j}(z_i)-y^M_{k,j,i}\right)^T \mathbf{V_y^{-1}} \left(y_{k,j}(z_i)-y^M_{k,j,i}\right) + \sum_{k=1}^{NS}\left(w_{k,NZ}-w^M_{k,NZ}\right)^T \mathbf{V_w^{-1}}\left(w_{k,NZ}-w^M_{k,NZ}\right)$$

Least-Squares

$$s.t.$$

$$\mathbf{F}_{k,j}\left[\frac{dy_{k,j}(z)}{dz}, y_{k,j}(z), w_{k,j}(z), z, \pi_{k,j}, \Pi\right]=0$$

$$\mathbf{G}_{k,j}\left[y_{k,j}(z), w_{k,j}(z), z, \pi_{k,j}, \Pi\right] 0$$

$$y_{k,j}(0)=\phi(y_{k,j-1}(z_{L_{k,j-1}}), F_{f_{k,j}})$$

$$j\in\{1..NZ\},\quad k\in\{1..NS\}$$

Rigorous Reactor Model

- **Special Case of Multi-Stage Dynamic Optimization Problem**
  - **Solve using Simultaneous Collocation-Based Approach**

1 data set		6 data sets
500 ODEs	x 6 →	3000 ODEs
1000 AEs		6000 AEs

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Large-Scale Parameter Estimation

- **Multi-Zone Tubular Reactor –** Quasi Steady-State
  - **Data Sets:** Operating Conditions and Properties for Different Grades
  - **Match:** Temperature Profiles and Product Properties
    - **On-line Adjusting Parameters** → Track Evolution of Disturbances
    - **Kinetic Parameters** → Development and Discrimination among Rigorous Models
- **Results**
  - **Single Data Set** (On-line Adjusting Parameters)

Grade	Constraints	Parameters	LB	UB	Iterations	CPUs	NZJ	NZH
A	11955	32	374	361	11	17.03	166425	87954
B	11283	32	374	361	8	10.06	138666	76890

  - **Multiple Data Sets** (On-line Adjusting Parameters + Kinetics)

Data Sets	Constraints	DOF	LB	UB	Iterations	CPUs	NZJ	NZH
3	33900	121	1246	1207	68	451.51	520275	552738
6	68421	217	2467	2389	58	900.21	1058412	1119258

Bottleneck (Memory Requirements)
Factorization Step

$$\begin{bmatrix} W(x_k,\lambda_k) & A(x_k) & -I \\ A(x_k)^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix}\begin{bmatrix}\Delta x\\ \Delta\lambda\\ \Delta\nu\end{bmatrix} = -\begin{bmatrix}\nabla f(x_k)+A(x_k)\lambda_k-\nu_k \\ c(x_k) \\ X_kV_ke-\mu_\ell e\end{bmatrix}$$

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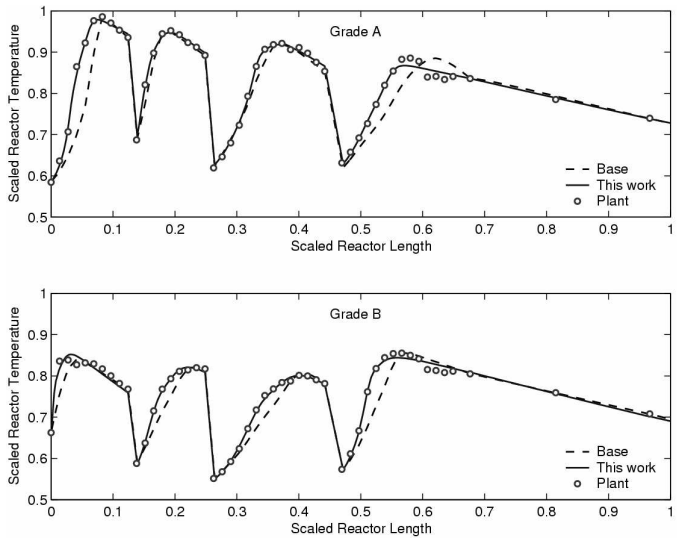
Large-Scale Parameter Estimation

Improved Match of Reactor Temperatures Profile



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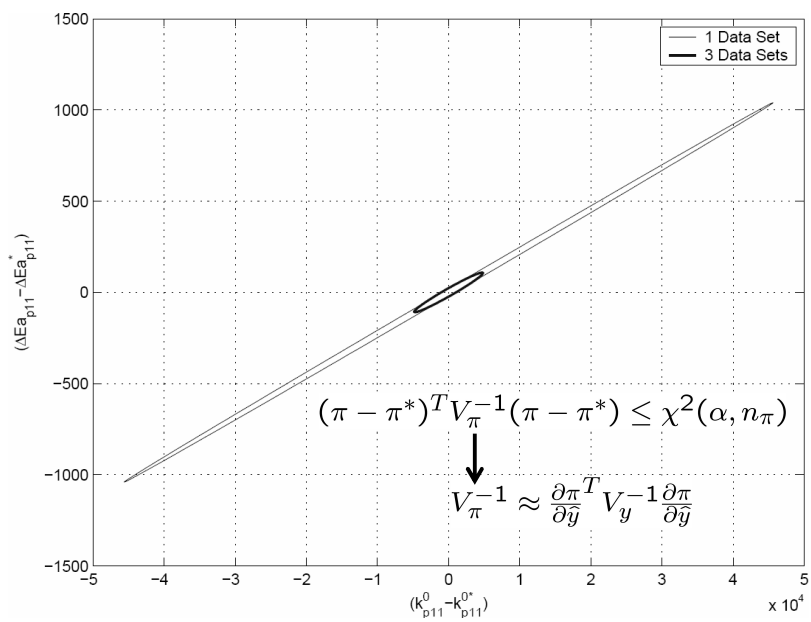
IPOPT Factorization Byproduct



$$(\pi - \pi^*)^T V_\pi^{-1} (\pi - \pi^*) \leq \chi^2(\alpha, n_\pi)$$

$$V_\pi^{-1} \approx \frac{\partial \pi}{\partial \hat{y}}^T V_y^{-1} \frac{\partial \pi}{\partial \hat{y}}$$

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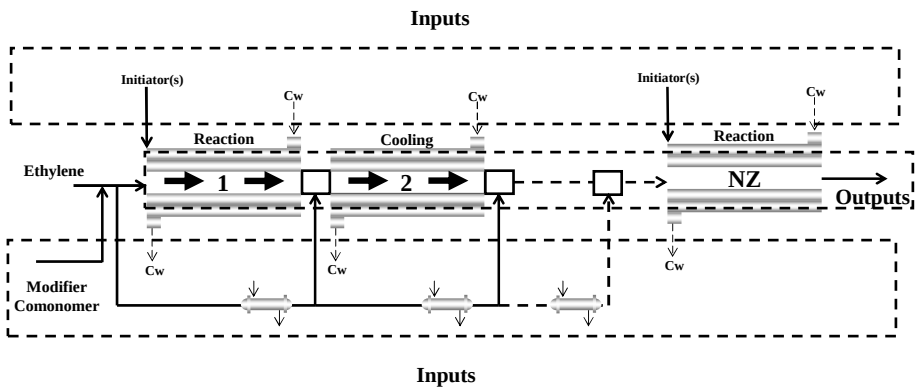
Advanced Regression Methods

Errors-In-Variables (EVM)

- **Standard Least Squares - Errors in Output Variables - *Biased* Parameters**
- **EVM - Errors in Output *AND* Input Variables - *Unbiased* Parameters**



Advanced Regression Methods

Errors-In-Variables (EVM)

EVM Drawback - Degrees of Freedom $DOF = \Pi + \sum_{k-1}^{NS}\sum_{j=1}^{NZ}\pi_{k,j} + \sum_{k=1}^{NS}\sum_{j=1}^{NZ}\sum_{i=1}^{NM_u(j)} u_{k,j,i}$

Formulation is Straightforward

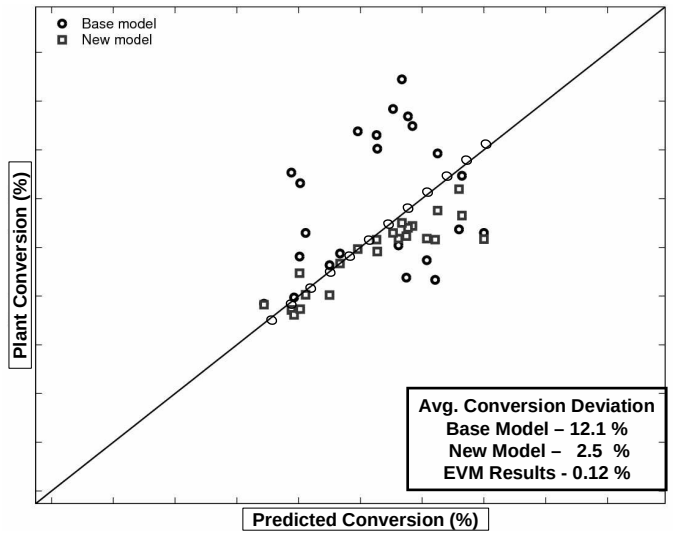
$$\min_{\Pi,\,\pi_{k,j},\,u_{k,j}} \sum_{k=1}^{NS}\sum_{j=1}^{NZ}\sum_{i=1}^{NM(j)} \left(y_{k,j}(z_i) - y^M_{k,j,i}\right)^T \mathbf{V_y^{-1}} \left(y_{k,j}(z_i) - y^M_{k,j,i}\right)$$
$$+ \sum_{k=1}^{NS} \left(w_{k,NZ} - w^M_{k,NZ}\right)^T \mathbf{V_w^{-1}} \left(w_{k,NZ} - w^M_{k,NZ}\right)$$
$$+ \sum_{k=1}^{NS}\sum_{j=1}^{NZ} \left(u_{k,j} - u^M_{k,j}\right)^T \mathbf{V_u^{-1}} \left(u_{k,j} - u^M_{k,j}\right)$$

EVM vs. Standard Least Squares

Data Sets	Constraints	DOF	LB	UB	Iterations	CPUs	NZJ	NZH
6 (EVM)	68627	529	2653	2575	71	1010.74	1059512	1119780
6 (SLS)	68421	217	2467	2389	58	900.21	1058412	1119258

Industrial Case Study

- **Results - Reactor Overall Monomer Conversion (up to 20 Different Grades)**



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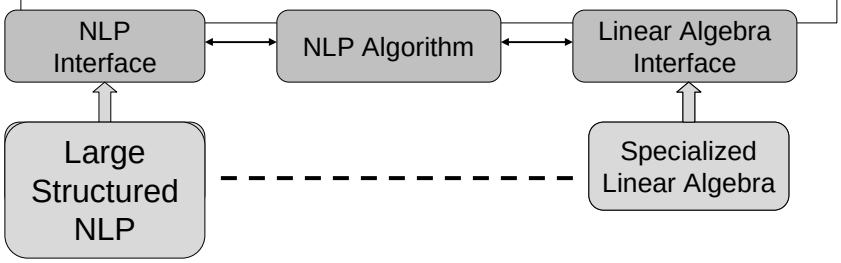
Next Generation IPOPT

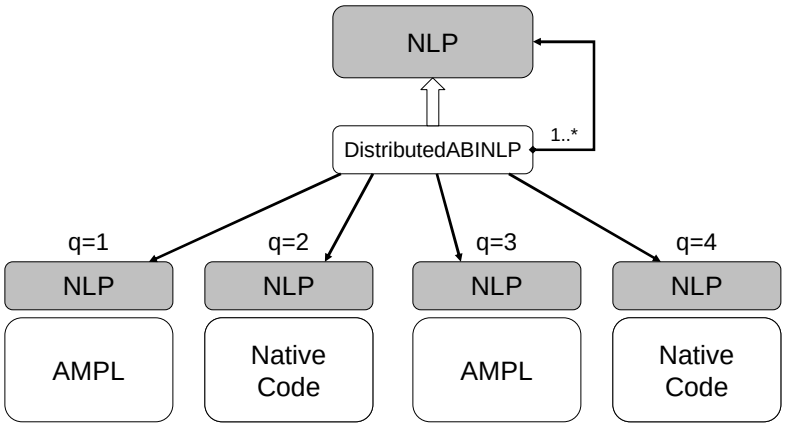
- IPOPT 3.2, Fall, 2006, CPL (www.coin-or.org)
  - Based on Fortran version
  - Object-oriented, NLP Solver
    - Primal-Dual Interior Point method
    - Full space - exact Hessian information
    - Monotone/Adaptive μ update
    - Filter line search strategy
  - Flexible algorithm structure
  - Interfacing to other linear solvers
  - Modeling Environments - AMPL, AIMMS, MATLAB…
- *Ideal for Internal Decomposition*
  - Consistent linear system structure at every iteration
  - Separation of algorithm and specialized linear algebra

High Level IPOPT Design



- Provide structured NLP elements
  - Hessian, jacobian, gradients, residuals, variables,
- Vector operations
  - BLAS, norms, dot products, axpy, element- wise, max, min, etc.
- Matrix-Vector operations
  - $M\,v$, $M^T v$
- Solution of Linear KKT system

Modeling the Block NLP



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Parameter Estimation in Parallel Architectures

Exploit Structure of KKT Matrix – *Laird, Biegler 2006*

$$\min_{\Pi,\pi_{k,j}} \sum_{k=1}^{NS}\sum_{j=1}^{NZ}\sum_{i=1}^{NM(j)} \left(y_{k,j}(z_i)-y^M_{k,j,i}\right)^T \mathbf{V}_{\mathbf{y}}^{-1}\left(y_{k,j}(z_i)-y^M_{k,j,i}\right) + \sum_{k=1}^{NS}\left(w_{k,NZ}-w^M_{k,NZ}\right)^T \mathbf{V}_{\mathbf{w}}^{-1}\left(w_{k,NZ}-w^M_{k,NZ}\right)$$

$$s.t.\quad \mathbf{F}_{k,j}\left[\frac{dy_{k,j}(z)}{dz}, y_{k,j}(z), w_{k,j}(z), z, \pi_{k,j}, \Pi\right]=0$$
$$\mathbf{G}_{k,j}\left[y_{k,j}(z), w_{k,j}(z), z, \pi_{k,j}, \Pi\right]=0$$
$$y_{k,j}(0)=\phi(y_{k,j-1}(z_{L_{k,j-1}}), F_{f_{k,j}})$$
$$j\in\{1..NZ\},\quad k\in\{1..NS\}$$

$$\begin{aligned} \min \quad & f(x) \\ \text{s.t.} \quad & c(x)=0 \\ & x\geq 0 \end{aligned}$$

$$\begin{aligned} \min \quad & \sum_{k=1}^{N_S} f_k(x_k) \\ \text{s.t.} \quad & c_k(x_k,\Pi)=0 \\ & x_k,\Pi\geq 0 \end{aligned}$$

$$\begin{bmatrix} H_k & A_k & -I \\ A_k^T & 0 & 0 \\ V_k & 0 & X_k \end{bmatrix}\begin{bmatrix} \Delta x \\ \Delta\lambda \\ \Delta\nu \end{bmatrix} = -\begin{bmatrix} r_x \\ r_\lambda \\ X_kV_ke-\mu_\ell e \end{bmatrix}$$

Direct Factorization MA27
Memory Bottlenecks
Factorization Time *Scales Superlinearly* with Data sets

$$\begin{bmatrix} \mathbf{K}_1 & & & & Q_1 \\ & \mathbf{K}_2 & & & Q_2 \\ & & \ddots & & \vdots \\ & & & \mathbf{K}_N & Q_N \\ Q_1^T & Q_2^T & \dots & Q_N^T & D_\Pi \end{bmatrix}\begin{bmatrix} \Delta s_1 \\ \Delta s_2 \\ \vdots \\ \Delta s_N \\ \Delta\Pi \end{bmatrix} = -\begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_N \\ r_\Pi \end{bmatrix}$$

Block-bordered Diagonal Structure
Coarse-Grained Parallelization

Parameter Estimation in Parallel Architectures

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$$\begin{bmatrix} \Delta s_1 \\ \Delta s_2 \\ \vdots \\ \Delta s_N \\ \Delta\Pi \end{bmatrix} = -\begin{bmatrix} r_1 \\ r_2 \\ \vdots \\ r_N \\ r_\Pi \end{bmatrix}$$

1) **Parallelizable**
Sparse Factorization $\mathbf{K}_i$ in each Block
Inertia Correction

2) **Non-parallelizable**
Dense Factorization of $\mathbf{S} \rightarrow dim\{\Pi\}$

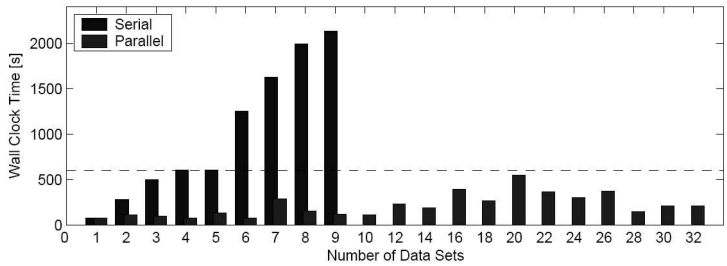
3) **Parallelizable**
Final Backsolve

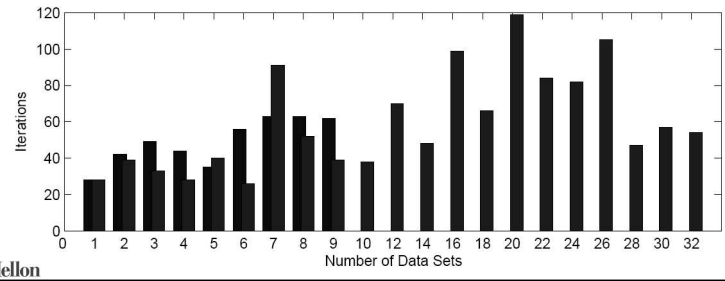
Parameter Estimation in Parallel Architectures

Computational Results – LDPE Reactor EVM Problem

Beowulf Cluster – ChemE Department, Carnegie Mellon University

Intel Pentium 4 Xeon 2.4ghz, 2gb RAM





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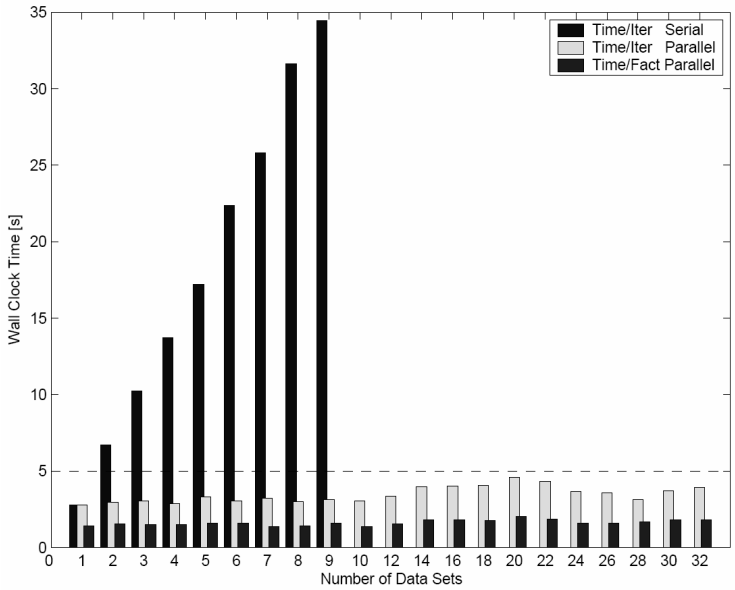
Parameter Estimation in Parallel Architectures

Computational Results – LDPE Reactor EVM Problem



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Conclusions – Parameter Estimation

- Trust Region (Levenberg-Marquardt) methods: standard for unconstrained problems - MINPACK, NaG, NL2SOL, Harwell
- Constrained problem formulations - more model flexibility
- SQP codes adapted to exploit least squares structure, faster methods
- EVM problems - expensive for conventional optimization codes
  - Many degrees of freedom for optimization
  - Decomposition of KKT conditions required
  - ODRPACK (netlib) developed for $y_u = f_u(\theta)$
- Large-scale SQP methods developed for:
  - Parameter estimation
  - EVM methods
  - Data Reconciliation
- IPOPT has useful characteristics for large-scale parameter estimation

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Optimization Algorithms for Data Reconciliation

Introduction to Data Reconciliation

M-Estimators
- Bayesian Forms
- Fair Function
- Redescending Estimator

Akaike Information Criterion

Mixed Integer Formulations

Static Examples

Dynamic Examples

Conclusions

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Introduction

- Data contaminated by errors
  - Random errors:
    - High frequency noise
    - Typically $\sim \mathcal{N}(0, \Sigma^2)$
  - Gross errors and outliers
    - Systematic occurrences: biases, drifts
    - Not modeled by distributions
- Contaminated data can bias estimates
- Difficult to converge NLP when data noisy
- Inputs may be contaminated

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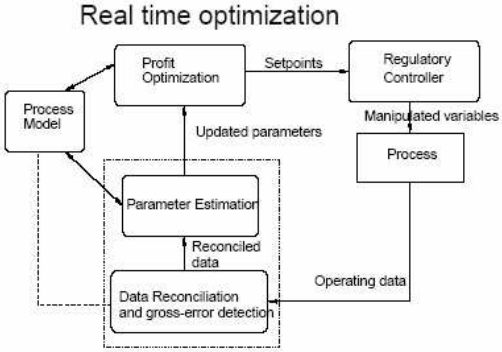
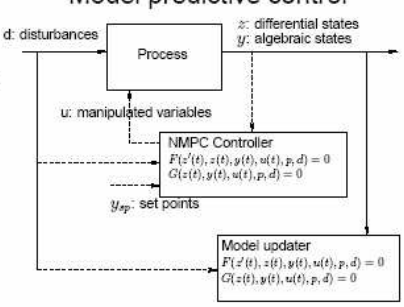
Data Reconciliation Framework

- Industrial applications of data reconciliation and parameter estimation (DRPE)

Real time optimization

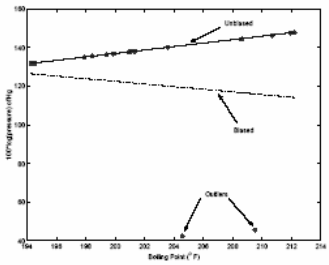


Model predictive control



Effects of Gross Error in Regression

Example: Boiling point of H_2O vs. atm. pressure with 2 outliers (Weisberg, 1985)



Sources of gross errors: Broken gauges, process leaks, improperly used measurement devices, operator errors

Identify and negate effects of gross errors

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Data Reconciliation – Literature Review

- Sequential χ^2 tests:
  - Crowe et al. (1983), Madron (1985), Kao et al. (1992)
- Combinatorial
  - Serth and Heenan (1986), Narasimhan and Mah (1987): Serial Combination and Generalized Likelihood Ratio tests
  - Crowe (1989): Max. power test
  - Rollins et al. (1996): Linear Combination Test based on χ^2 tests
  - Bagajewicz et al. (1998): Graph theory based, linear ODEs
- Simultaneous
  - Tjoa and Biegler (1991): Contaminated normal - difficult to tune, cannot detect biases
  - Albuquerque and Biegler (1996): Fair function - easy to use, no explicit outlier identification

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Treatment of Outliers: M-Estimators

M-Estimator: modeling the influence of residual outliers through modification of maximum likelihood (ML) functions

Bayesian Statistics and Bernoulli Trials

- Statistical definitions and ML function
- Allows statistical inference

Robust Statistics

- Modification without inferential aspects

Akaike Information Criterion (AIC)

- Based on ML extended to discrete parameters

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Bayesian Approach: Bernoulli Trial

Assume separate probability distributions for random and gross errors:

$$P(\varepsilon_i \mid \theta, X_i) = R(\varepsilon_i \mid \theta, X_i)\Pi(R) + G(\varepsilon_i \mid \theta, X_i)\Pi(G)$$

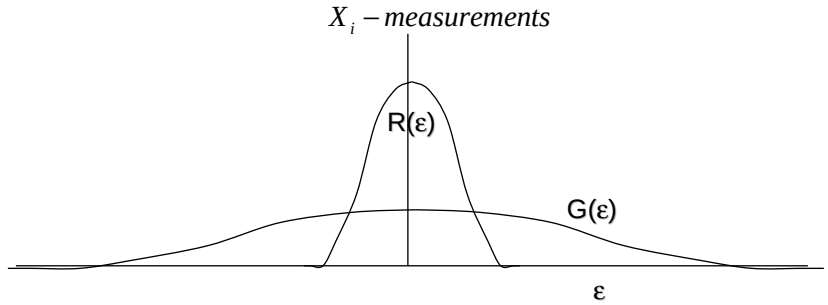
$$P, R, G - \text{ probability distributions}$$

$$\Pi(R), \Pi(G) - \text{ prior distributions}$$

$$\varepsilon_i \text{- measurement error}$$

$$\theta - \text{ parameters}$$

$$X_i - \text{measurements}$$



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Bayesian Approach: Bernoulli Trial

Combine both distributions into ML function:

$$P(\varepsilon_i \mid \theta, X_i) = R(\varepsilon_i \mid \theta, X_i)\Pi(R) + G(\varepsilon_i \mid \theta, X_i)\Pi(G)$$

$$P(\varepsilon_i \mid \theta, X_i) = R(\varepsilon_i \mid \theta, X_i)(1-p) + G(\varepsilon_i \mid \theta, X_i)\,p$$

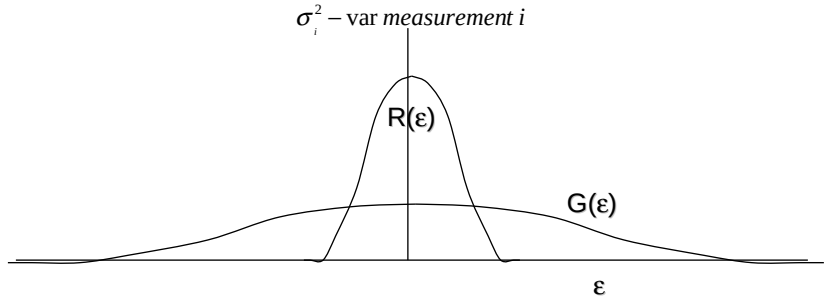
$$P(\varepsilon_i \mid \theta, X_i) = \exp(-\varepsilon_i^2/\sigma_i^2)(1-p)/\sigma_i + \exp(-\varepsilon_i^2/(b\sigma_i)^2)\,p/(\sigma_i b)$$

$$\max \sum_i \log(P(\varepsilon_i \mid \theta, X_i))$$

$$p \text{ - } fraction\ gross\ errors$$

$$b - \ scale\ of\ distributions$$

$$\sigma_i^2 - \text{var}\ measurement\ i$$

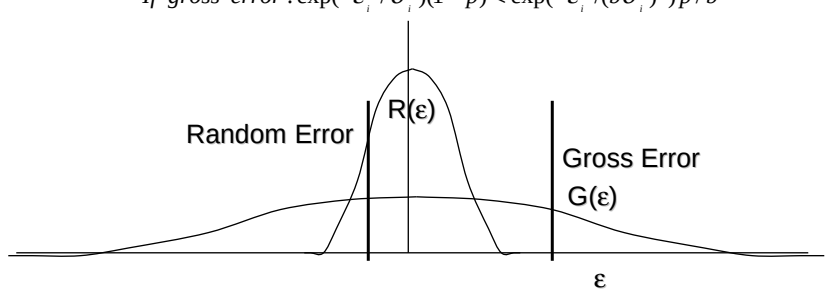


Bayesian Approach: Gross Error Test

Solve optimization problem and perform gross error tests at solution:

$$\max \sum_i \log(\exp(-\varepsilon_i^2/\sigma_i^2)(1-p) + \exp(-\varepsilon_i^2/(b\sigma_i)^2)\,p/b)$$

$$If\ \ gross\ \ error: \exp(-\varepsilon_i^2/\sigma_i^2)(1-p) < \exp(-\varepsilon_i^2/(b\sigma_i)^2)\,p/b$$



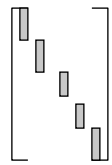
+ Statistical basis for determining gross errors
-Assumes gross errors follow proposed distribution
-Not robust to deviations from assumptions

Example (Pai and Fisher, 1988)

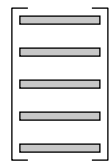
$$0.5(x_1)^2 - 0.7x_2 + x_3u_1 + (x_2)^2u_1u_2 + 2x_3(u_3)^2 - 255.8 = 0$$
$$x_1 - 2x_2 + 3x_1x_2 - 2x_2u_1 - x_2u_2u_3 + 111.2 = 0$$
$$x_3u_1 - x_1 + 3x_1x_3 - 2x_2u_1 - x_2u_2u_3 + 111.2 = 0$$
$$x_4 - x_1 - (x_3)^2 + u_2 + 3u_3 = 0$$
$$x_5 - 2x_3u_2u_3 = 0$$
$$2x_1 + x_2x_3u_1 + u_2 - u_3 - 126.6 = 0$$

5 measured variables (x)
3 unmeasured variables (u)
b= 20, p=0.2, σ=0.1

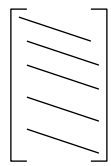
Introduce 20% gross error into
500 data sets generated randomly



100 right
0 wrong



87 right
0 wrong



99 right
1 wrong

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Robust Statistics for Gross Errors

- Common Assumption: Data with normally distributed random errors ⇒ likelihood function is *least squares estimator*
- likelihood of data corrupted with outliers: difficult to determine
- Estimators derived from fixed probability distribution: not justified
- Robust Estimators:
  - largely distribution independent
  - unbiased estimates when data from ideal distribution
  - Insensitive to deviations from ideality
  - Add less weight to outlying measurements ⇒ *protect* other measurements from being corrupted

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Robust Statistics Properties

Find estimators that are insensitive to deviations in assumptions of noise distribution.

F – assumed distribution of data

G – actual distribution of data

$$\delta(F,G) < \varepsilon \Rightarrow \delta(T(F),T(G)) < \gamma$$

T(-) – test statistic or distribution of estimator

<u>Example:</u>

S1: [2.0, 2.1, 2.2, 2.3, 2.4] Mean = 2.2, Median=2.2

S2: [2.0, 2.1, 2.2, 2.3, 24] Mean = 6.56, Median=2.2

➔ Median is a robust statistic, Mean is not.

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Huber Class of Robust Estimators (1981)

Fair Function (Rey, 1988)

$$\rho_{Fi} = C^2\left[\frac{|\varepsilon_i|}{C} - \log\left\{1+\frac{|\varepsilon_i|}{C}\right\}\right]$$

- Use $\sum_i \rho_{Fi}$ instead of least squares objective
- Convex function of <u>normalized</u> residual
- Small residuals – quadratic behavior
- Large residuals – linear behavior
- C – Tuning parameter based on Cramer-Rao bound (trade off efficiency (high C) with robustness (low C))

$$C = 0.21529\left(\frac{\varphi - 0.63662}{1-\varphi}\right) \quad where \quad \varphi = \frac{\sigma^2}{V_{Fair}}$$

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Hampel Class of Robust Estimators

Three Part Redescending Estimator (Hampel, 1974)

$$\rho_{H_i} = \begin{cases} \frac{1}{2}\varepsilon_i^2, & 0 \le |\varepsilon_i| \le a \\ a\,|\varepsilon_i| - \frac{a^2}{2}, & a < |\varepsilon_i| \le b \\ ab - \frac{a^2}{2} + (c-b)\frac{a}{2}\left[1 - \left(\frac{c-|\varepsilon_i|}{c-b}\right)^2\right], & b < |\varepsilon_i| \le c \\ ab - \frac{a^2}{2} + (c-b)\frac{a}{2}, & |\varepsilon_i| > c, \end{cases}$$

Three parameters define regions: c > b+2a

Quadratic, linear and constant parts involving normalized residual

Nonsmooth – requires some smoothing approximations

Not clear how to tune a, b, c

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M-Estimators in Robust Statistics

M-Estimators

- Overall likelihood of N observations: $\mathcal{L} = \prod_{i=1}^{N} \ell(x_i|p)$
- M-estimator = $\rho^M = -log\ \mathcal{L} = -\sum_{i=1}^{N} log\ \ell(x_i|p)$

M-Estimators Used $\mathcal{IF} = \psi(\varepsilon_0) = \lim_{t\to 0} \frac{T[(1-t)f + t\delta(\varepsilon - \varepsilon_0)] - T[f]}{t}$

1. Least Squares Estimator (Non robust)
   - Severely biased by outliers
2. Fair Function (Robust)
   - $\mathcal{IF}$ is bounded as $\varepsilon \to \infty$
3. Three part Redescending Estimator (Robust)
   - $\mathcal{IF} \to 0$ as $\varepsilon \to \infty$

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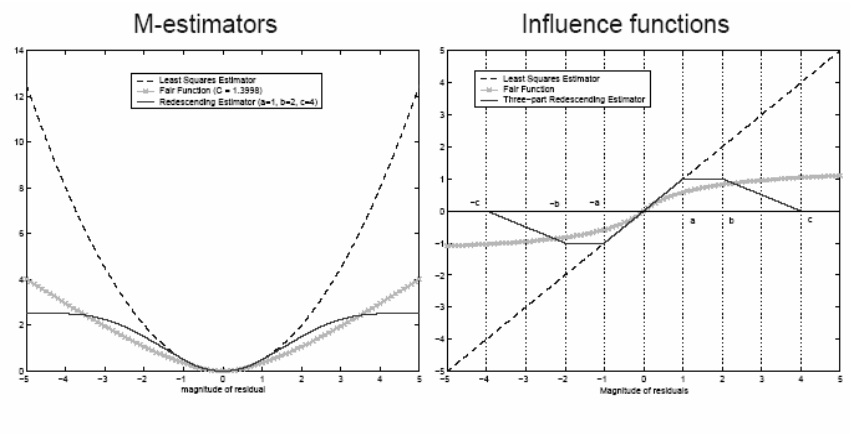
Properties of M-Estimators



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Properties of M-Estimators

	Bayesian	Robust
Distributional Assumptions?	Yes	No
Sensitive to Assump. Deviations?	Yes	No
Statistical Inference at Solution?	Yes	No
Incorporate prior knowledge?	Yes	No

-For robust case, apply exploratory statistics (e.g., boxplots) at solution

- Need data redundancy to identify gross errors

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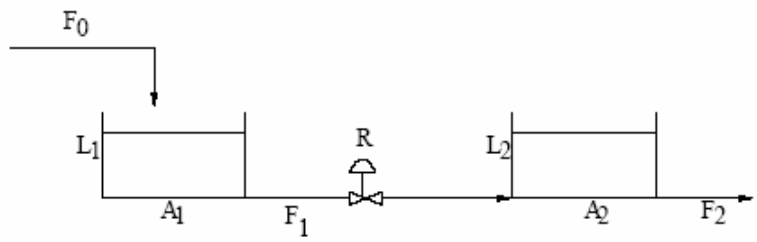
Dynamic Data Reconciliation



- Measurements: Flows F_0, F_1, F_2 & heights L_1 and L_2
- DAE system
- Parameters: Tank areas: $1/A_1$ & $1/A_2$

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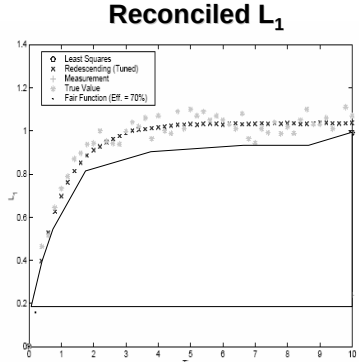
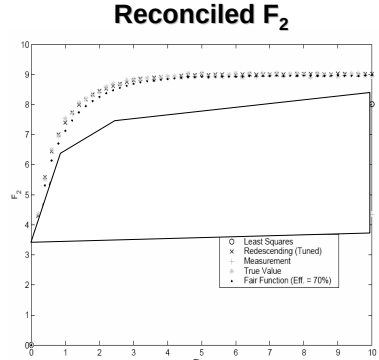
Case 1: Comparison of Results

Reconciled L_1



Reconciled F_2



•Discretize DAEs and solve as large scale NLP problem with appropriate objective function

•Add random outlier noise to flow and level data

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Tank Example – Case 1

- Outliers drawn from broad random distribution (distributional assumption satisfied)
- Data reconciliation and parameter estimates done well by
- Bayesian approach and M-estimators

Parameters	$1/A_1$	$1/A_2$
True Values	0.5	0.5
Least Squares	0.698	0.503
Bayesian	0.490	0.50
Fair Function	0.501	0.501
Redesc. Tuned	0.50	0.50

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Tank Example – Case 2

- Outliers systematic (distributional assumption violated); measurements for L_1 and F_2 stuck
- Data reconciliation and parameter estimation poor with Bayesian approch
- Data reconciliation does and parameter estimates done better by
- M-estimators

Parameters	$1/A_1$	$1/A_2$
True Values	0.5	0.5
Least Squares	0.25*	0.55
Bayesian	0.25	0.25
Fair Function	0.25	0.439
Redesc. Tuned	0.499	0.500

*lower bound

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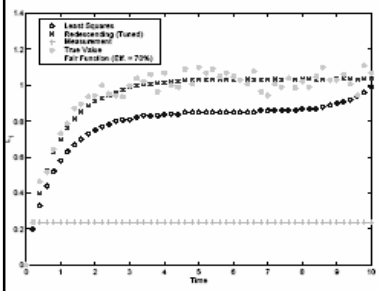
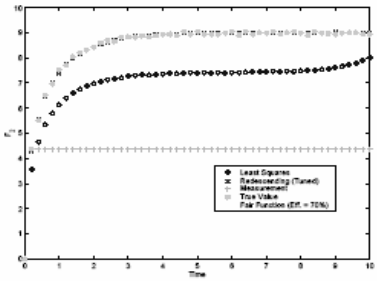
Case 2: Comparison of Results

Reconciled L_1



Reconciled F_2



- Least squares: Very poor DRPE
- Fair function: Better than least squares but inadequate
- Redescending: Avoids bounds on $1/A_1$ and $1/A_2$. Tuned for best result

Redescending Estimators superior for problems with largely corrupted data

Gross Errors Modeled with AIC

Common statistical framework for combinatorial and robust DRPE strategies?

- DR & Gross error detection $\equiv$ model discrimination and PE
- Data models $\Rightarrow$ partitions of residuals into random and gross errors
- Parameters = # of outliers + model parameters
- Obtain most likely model and its parameters
- Max. likelihood estimators (MLE): asymptotically efficient $\Rightarrow$ likelihood function = sensitive criterion of deviation of parameters from true values
- Akaike Information Criterion ($\mathcal{AIC}$): Distance between fitted and true models

$$\mathcal{AIC} = -2 \cdot \log(\text{maximum likelihood}) + 2(\text{\# independently adjusted parameters in model})$$

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AIC for Data Reconciliation

Objective Function

$$\mathcal{AIC} = -2log(\text{maximum likelihood}) + 2(\#\text{ independently adjusted parameters within the model}) .$$

$$\mathcal{AIC} = E(S) = 2\sum_{i=1}^{N} -log(\ell(\varepsilon(i,p),i,p)) + 2\ dim(p),$$

- **Contains discrete and continuous variables**
- **dim(p) = # gross errors in problem**
- **Leads to MINLP problem**
- **Can be simplified to MILP for linear systems**
- **AIC can also be used as an off-line objective for calibration**

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MINLP formulation

(Yamamura et al, 1988; Arora and B, 2001)

$$\min_{\substack{x_i,\mu_i,\\ y_i,z_i}} \sum_{i=1}^{n} \left[(x_i^M - x_i)/\sigma_i - \mu_i/\sigma_i\right]^2 + 2\cdot\sum_{i=1}^{n} y_i$$

$$\text{s.t. } \boxed{Ax = 0}$$

$$\mu_i \le U_i y_i$$

$$-\mu_i \le U_i y_i$$

$$\mu_i - z_i U_i - z_i L_i + L_i y_i \le 0$$

$$-\mu_i + z_i U_i + z_i L_i + L_i y_i \le L_i + U_i$$

$$x_i \ge 0$$

$$z_i \le y_i$$

$$y_i, z_i \in \{0,1\}.$$

-Direct minimization of AIC function

-Model is for linear system, but straightforward extension for nonlinear systems

- μ_i = positive or negative biases, $U \ge |\mu_i| \ge L$

-Binary variables enforce this:

y = 0,1: existence of gross error

z = 0,1: positive or negative sign

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MILP Simplification
(Soderstrom et al., 2000)

$$\min_{\substack{x_i,\mu_i,\\ y_i,z_i}} \sum_{i=1}^{n} \left|(x_i^M - x_i)/\sigma_i - \mu_i/\sigma_i\right| + \sum_{i=1}^{n} w_i \cdot y_i$$
$$\begin{aligned}
\text{s.t.}\quad & Ax = 0\\
& \mu_i \le U_i y_i\\
& -\mu_i \le U_i y_i\\
& \mu_i - z_i U_i - z_i L_i + L_i y_i \le 0\\
& -\mu_i + z_i U_i + z_i L_i + L_i y_i \le L_i + U_i\\
& z_i \le y_i\\
& y_i, z_i \in \{0,1\},
\end{aligned}$$

$$\min_{\substack{x_i,\mu_i,\\ y_i,z_i}} \sum_{i=1}^{n} (r_i + q_i)/\sigma_i + \sum_{i=1}^{n} w_i \cdot y_i$$
$$\begin{aligned}
\text{s.t.}\quad & Ax = 0\\
& x_i^M - (x_i + \mu_i) = r_i - q_i\\
& \mu_i \le U_i y_i\\
& -\mu_i \le U_i y_i\\
& \mu_i - z_i U_i - z_i L_i + L_i y_i \le 0\\
& -\mu_i + z_i U_i + z_i L_i + L_i y_i \le L_i + U_i\\
& z_i \le y_i\\
& r_i, q_i \ge 0\\
& y_i, z_i \in \{0,1\}.
\end{aligned}$$

- Quadratic terms become absolute values (like Huber)
- Weighting values (w_i) not clear
- Limited to linear models
- Much faster solution times

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Mixed Integer Formulation for Gross Errors

Minimize $\mathcal{AIC}$ by solving *MINLP*:

$$\begin{aligned}
\min_{x_i,\mu_i,y_i} \quad & \sum_{i=1}^{n} \left[\frac{(x_i^M - x_i)}{\sigma_i} - \frac{\mu_i}{\sigma_i}\right]^2 + 2 \cdot \sum_{i=1}^{n} y_i\\
\text{s.t.} \quad & Ax = 0, \qquad (-1)\\
& |\mu_i| \le U_i y_i,\\
& |\mu_i| \ge L_i y_i,\\
& y_i \in \{0,1\},\\
& x_i \ge 0.
\end{aligned}$$

MILP (Soderstrom et al., 2000):

$$\begin{aligned}
\min_{x_i,\mu_i,y_i} \quad & \sum_{i=1}^{n} \left|\frac{(x_i^M - x_i)}{\sigma_i} - \frac{\mu_i}{\sigma_i}\right| + \sum_{i=1}^{n} w_i \cdot y_i\\
\text{s.t.} \quad & Ax = 0, \qquad (-2)\\
& |\mu_i| \le U_i y_i,\\
& |\mu_i| \ge L_i y_i,\\
& y_i \in \{0,1\},\\
& x_i \ge 0.
\end{aligned}$$

w_i to obtain independent biases

- Both MINLP and MILP: Expensive for EVM problems
- In MILP: Choosing weights not entirely clear
- Neither suitable for large EVM problems

Cheaper + reliable DRPE in presence of outliers $\Rightarrow$ use Robust Statistics

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Tuning the Redescending Parameters

- Idea: *Minimize* $\mathcal{AIC}$ associated with the redescending estimator
- Tuning constants related to contamination in data
- Use size of redescending region to assign b and a to obtain c from $c = b + 2a$
- Simple Two-Step Tuning Procedure

1. Select range of redescending estimators 2. Perform DRPE and obtain values of $\mathcal{AIC}$	Step 1
3. Obtain bounds for location of minimum 4. Golden section search for c 5. $b = c/2$, $a = (c - b)/2$	Step 2

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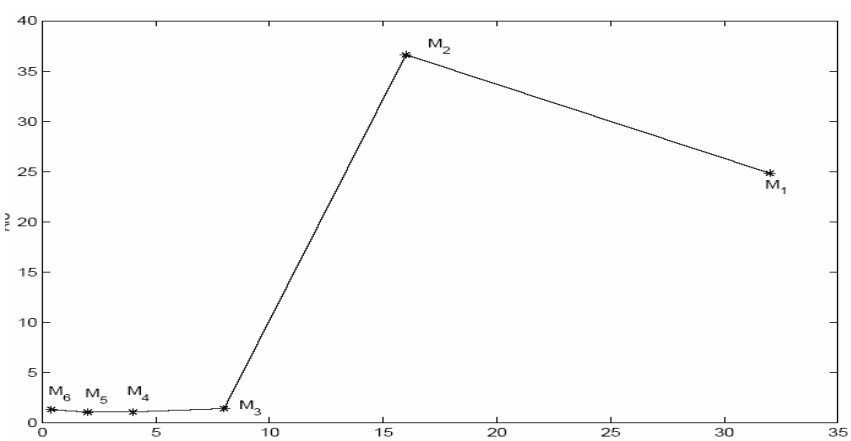
Tune Redescending Estimator Using AIC Tanks Example



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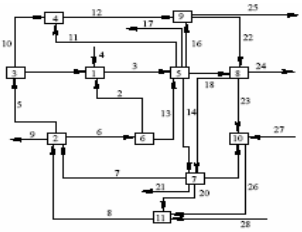
Steam Metering Example



- 28 streams, 11 nodes $\Rightarrow$ 11 linear equalities, 28 variables
- *Moving horizon* of data used $X^M = \begin{bmatrix} x_{11}^M & x_{12}^M & \cdots & x_{1H}^M \\ x_{21}^M & x_{22}^M & \cdots & x_{2H}^M \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1}^M & x_{n2}^M & \cdots & x_{nH}^M \end{bmatrix}$
- Sizes of horizon attempted: 5, 10, 20, 40
- 3, 5, 7 streams biased; bias propagation
- 100 moving horizons for fixed location of bias
- *Smoothed* redescending estimator for use in *GAMS*

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Steam Metering Results

$$\mathbf{OP} = \frac{\text{\# biases correctly identified}}{\text{\# biases simulated}}, \quad \mathbf{AVT1} = \frac{\text{\# unbiased wrongly identified}}{\text{\# simulation trials}}.$$

Sample results for horizon size = 5, 3 biases:

Method	$\mathbf{w_i}$	OP	AVT1	$\mathcal{AIC}$	CPU (s)/ horizon
Fair function	–	0.640	3.907	–	–
RE (a, b, c)					
0.5, 1, 2	–	0.673	5.820	3.491	1.114
1, 2, 4	–	0.626	2.065	14.112	1.075
2, 4, 8	–	0.571	0.305	40.299	1.057
4, 8, 16	–	0.455	0.069	96.399	1.019
MINLP	–	0.885	0.071	1.067	42.989
MILP	1	0.685	2.265	1.211	4.369
MILP	$2H$	0.704	0.081	1.117	0.592
MILP	100	0.112	0.000	17.148	0.386

- MIPs: used info. abt. type of gross error; EVM too expensive
- RE tailored to process $\Rightarrow$ Tune RE parameters to minimize $\mathcal{AIC}$

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Conclusions – Data Reconciliation

- Redescending estimators superior for gross error detection and provide good parameter estimates
- Redescending estimators
  - More robust than Huber estimator: Fair function
  - Can be tuned
- Simple two-step tuning strategy utilized: considerably improves DRPE
- MINLP and MILP: good but computationally intensive and useful only for linearly constrained problems

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